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ENV/IT/000167

***Toxeraser*:**
the tool for substitution specifically designed for the cosmetic sector

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Action B5: Building the SPHERA risk assessment tool with the capacity to integrate risk factors into a single decision-making index

Task B.5.2. The ToxEraser concept

- a set of molecules matching the functional category can be retrieved along with its classification in terms of safety (see Table of *Cosmetics according to safety*):

- further details can be also appreciated:

  a) the specific US institution providing the safety response
  b) the molecules' identifier (SMILES, CAS, IUPAC name)

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Task B.5.2. The ToxEraser concept

- **Systematic retrieval of information about cosmetics, concerning:**
  - **safety**
  - **functional uses**

Task B.5.1. Definition of the libraries of parameters to characterize safety

The 'Cosmetics' case study

Existing exclusion list

- SIN list
- Substances not allowed or restricted in cosmetics (Annexes of the Cosmetic Regulation 1223/2009)
- CMR from COSING

Existing safer chemicals list

- Safer Chemical Ingredient List (SCIL)
- Generally Recognized As Safe (GRAS)
- Allowed in the European market

Other lists

- CIR (Cosmetic Ingredient Review)
- IFRA (International Fragrance Association)

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Cosmetics ingredients databases characteristics:

- information covers an extensive range of toxicological endpoints and environmental fate data
- assessed endpoints depend also on the functional category of the cosmetic (for instance, skin sensitization represents a main concern for fragrances)
- information is extracted by considering distinct line of evidence (toxicokinetic toxicological, carcinogenicity studies, reproductive toxicity, dermal, ocular and mucosal irritation and sensitization)
- evaluation covers both experimental and *in silico* approaches, whereby '*in vivo'* evidence 'weights' more than results of '*in vitro'* and '*in silico'* assessment
- when based on the evaluation of dossiers on chemical ingredient, the manufacturer is supposed to disclose all product ingredients
- in some cases, information derives from an extensive search of the world literature
- furthermore, an ingredient regarded as generally safe can also be an ingredient that has been allowed in the marked without causing any harm

Cosmetics according to safety

meta-classes labels	Rank	N
regarded as generally safe	*1*	456
regarded as generally safe with restrictions	*2*	412
only commercially available	*3*	385
only commercially available with restrictions	*4*	565
banned or not recommended	*5*	417

Cosmetics according to safety

Class A labels	Class B labels	meta-classes labels	Rank	N
US and UE	*allowed without restrictions*	regarded as generally safe	*1*	456
	allowed with restrictions	regarded as generally safe with restrictions	*2*	412
Only UE	*allowed without restrictions*	only commercially available	*3*	385
	allowed with restrictions	only commercially available with restrictions	*4*	565
	banned or not recommended	banned or not recommended	*5*	417

Cosmetics according to safety

Class A labels	Class B labels	meta-classes labels	Rank	N	Cosing N(%)	CMR N(%)	SCIL N(%)	CIR N(%)	SCOGS N(%)	IFRA N(%)
US and UE	*allowed without restrictions*	regarded as generally safe	*1*	456	152 (33.33)	0	181 (39.69)	339 (74.34)	14 (3.07)	0
	allowed with restrictions	regarded as generally safe with restrictions	*2*	412	175 (42.48)	38 (9.22)	38 (9.22)	404 (98.06)	8 (1.19)	4 (0.97)
Only UE	*allowed without restrictions*	only commercially available	*3*	385	385 (100)	0	0	0	0	0
	allowed with restrictions	only commercially available with restrictions	*4*	565	503 (89.03)	81 (14.34)	0	0	0	102 (18.05)
	banned or not recommended	banned or not recommended	*5*	417	215 (51.56)	218 (52.28)	0	25 (6.00)	0	68 (16.31)
total	2235	1430 (63.98)	337 (15.08)	219 (9.80)	768 (34.36)	22 (1.94)	174 (7.79)			

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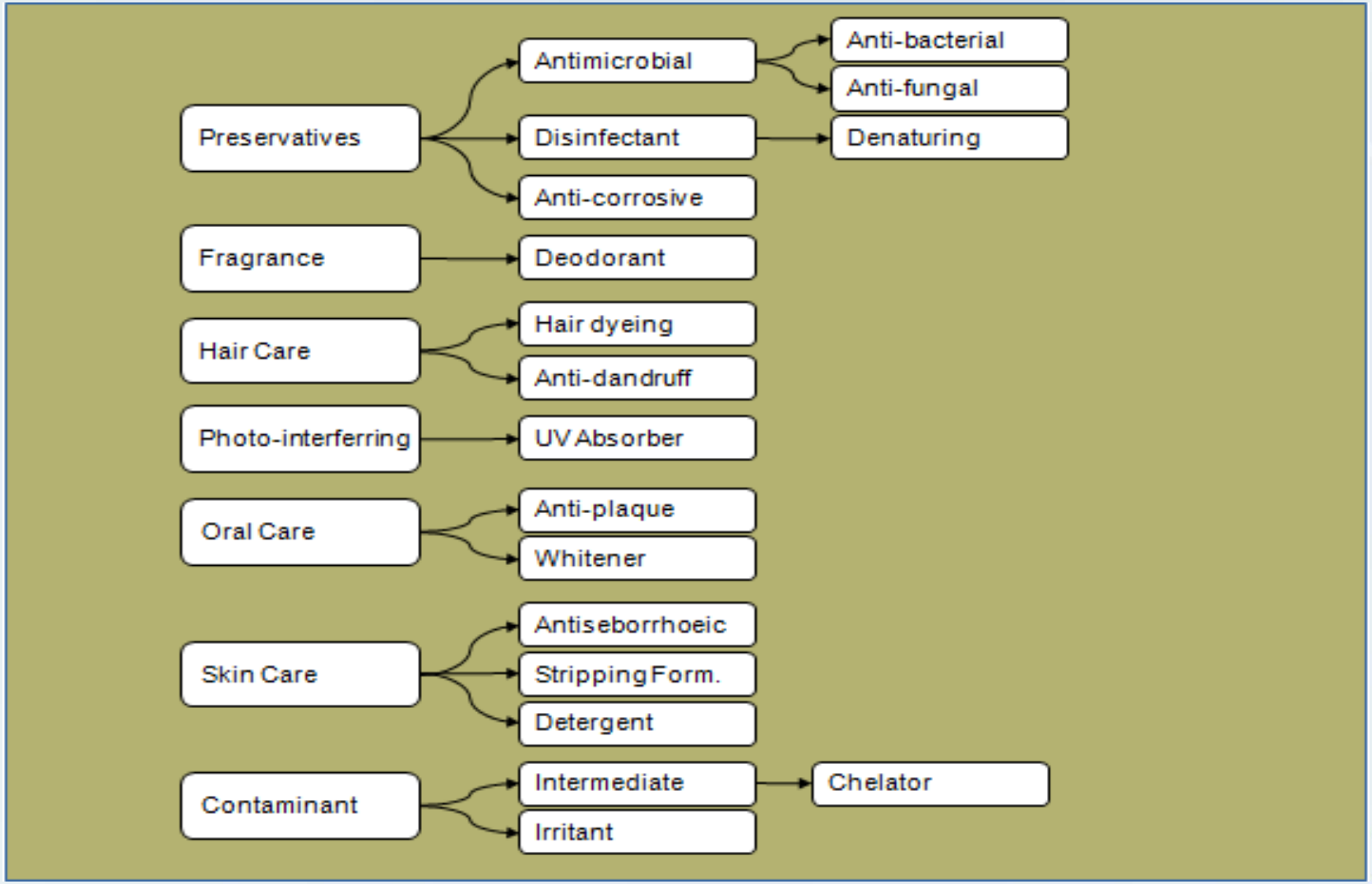
Cosmetics according to their functional uses: the hierarchical ontology



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Task B.5.2. The ToxEraser concept

Substitute a cosmetic with a safer one

The user is expected to specify the cosmetic functional category of interest.
To facilitate the search, the **functional category ontology** covers both:

a) the relationships between generic and specific labels

b) synonyms referred to the same category